Fluid Mechanics, Heat Transfer, and Thermodynamics Design Project

Production of Acrylic Acid

We are investigating the feasibility of constructing a new, grass-roots, 50,000 metric tons/year, acrylic acid production facility. As part of the feasibility study, we would like you to investigate some of the details of the feed and reaction sections of the proposed plant.

Acrylic Acid Production Reactions

The reactions are given below. The primary reaction is:

$$C_3H_6 \quad + \quad 1.5O_2 \;\rightarrow\; \underset{\text{acrylic acid}}{C_3H_4O_2} \quad + \quad H_2O \tag{1}$$

The secondary reactions are:

$$C_3H_6 \quad + \quad 2.5O_2 \;\rightarrow\; \underset{\text{acetic acid}}{C_2H_4O_2} \quad + \quad CO_2 \quad + \quad H_2O \tag{2}$$

$$C_3H_6 \quad + \quad 4.5O_2 \;\rightarrow\; 3CO_2 \quad + \quad 3H_2O \tag{3}$$

For the purposes of this preliminary evaluation, it is assumed that the reactions occur in a fluidized bed of catalyst particles. Due to the characteristics of fluidized bed reactors, a maximum propylene conversion of 90% is possible in the reactor. The selectivity for acrylic acid/acetic acid is 13.5. The selectivity for acrylic acid/carbon dioxide formed in the combustion reaction (Reaction (3)) is 1.6.

Reaction Section

The PFD for the reaction section is given in Figure 1. The propylene is stored in tanks which are not shown. There are two tanks, each holding a one-day supply, one in a filling mode and the other in a feeding mode. The propylene is stored at ambient temperature (which may be assumed to be 25°C) as a vapor/liquid equilibrium mixture, and the feed to the process may either be vapor (drawn from the top of the tank) or liquid (drawn from the bottom of the tank). The feed to the reactor must be at 4.3 bar and the crude acrylic acid product (in the liquid phase) may not exceed 90°C. The pressure drops across process units at base case

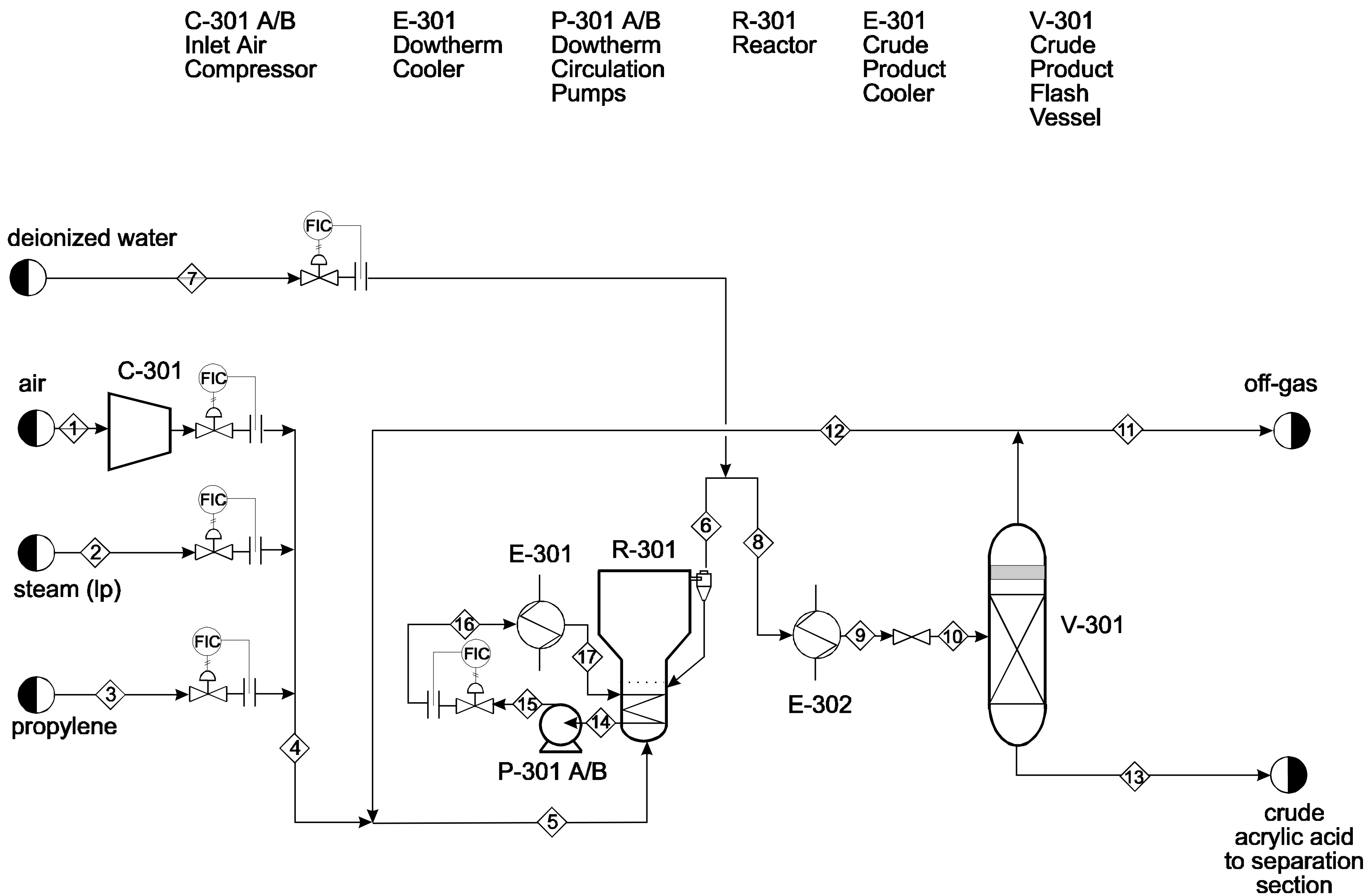


Figure 1: PFD for Unit 300 - Acrylic Acid from Propylene

conditions are given in Table 1.

Table 1: Pressure Drops across Process Units in Feed Section

Unit	ΔP (bar)
mixing points	0.05
Reactor	0.80
any heat exchanger	0.35

The reactor feed must be at 4.3 bar and 190°C. Heat generated in the reactor is removed by Dowtherm A™, which is thermally regenerated in E-301. If the Dowtherm pressure is maintained above 10 bar, it is not volatile up to 400°C. The reactor exit temperature is 290°C. Following the reactor, the reaction products are quenched with sufficient deionized water to bring the temperature of the stream to 200°C. The crude acrylic acid product is obtained by flashing the quenched reactor effluent. It may be assumed that all light gases (N_2, O_2, CO_2) leave in the vapor phase. All other components distribute between the vapor and liquid phases. The temperature of any liquid stream containing acrylic acid may never exceed 90°C to avoid spontaneous polymerization.

Assignment

Your assignment consists of three "mini-designs."

1. **Optimization of the Feed Section.** (ChE 110(fluids) and 142(thermo)) Refer to Figure 1. You are to determine the optimum pipe sizes for Streams 1-4. Equivalent pipe lengths can be determined from the attached plot plan (Figure 2). Pipe runs are at 4 m elevation off the ground, and you should add 90° elbows as necessary. The objective function is the Equivalent Annual Operating Cost (EAOC) of the feed section ($/y). The *EAOC* is defined as:

$$EAOC = CAP\left(\frac{A}{P}, i, n\right) + \text{operating costs for feed section loop} \tag{4}$$

where *CAP* = the installed cost of equipment in the feed section and

$$\left(\frac{A}{P}, i, n\right) = \frac{i(1+i)^n}{\left[(1+i)^n - 1\right]} \tag{5}$$

where i = 0.15 (15% rate of return) and n = 10 (ten year plant life).

For the feed section, do not include tank costs, so *CAP* includes the cost of pipes, pumps (if needed), and compressors and operating costs include the electricity to run the pumps and/or compressors. You are also to size and cost the feed tanks (1 day of

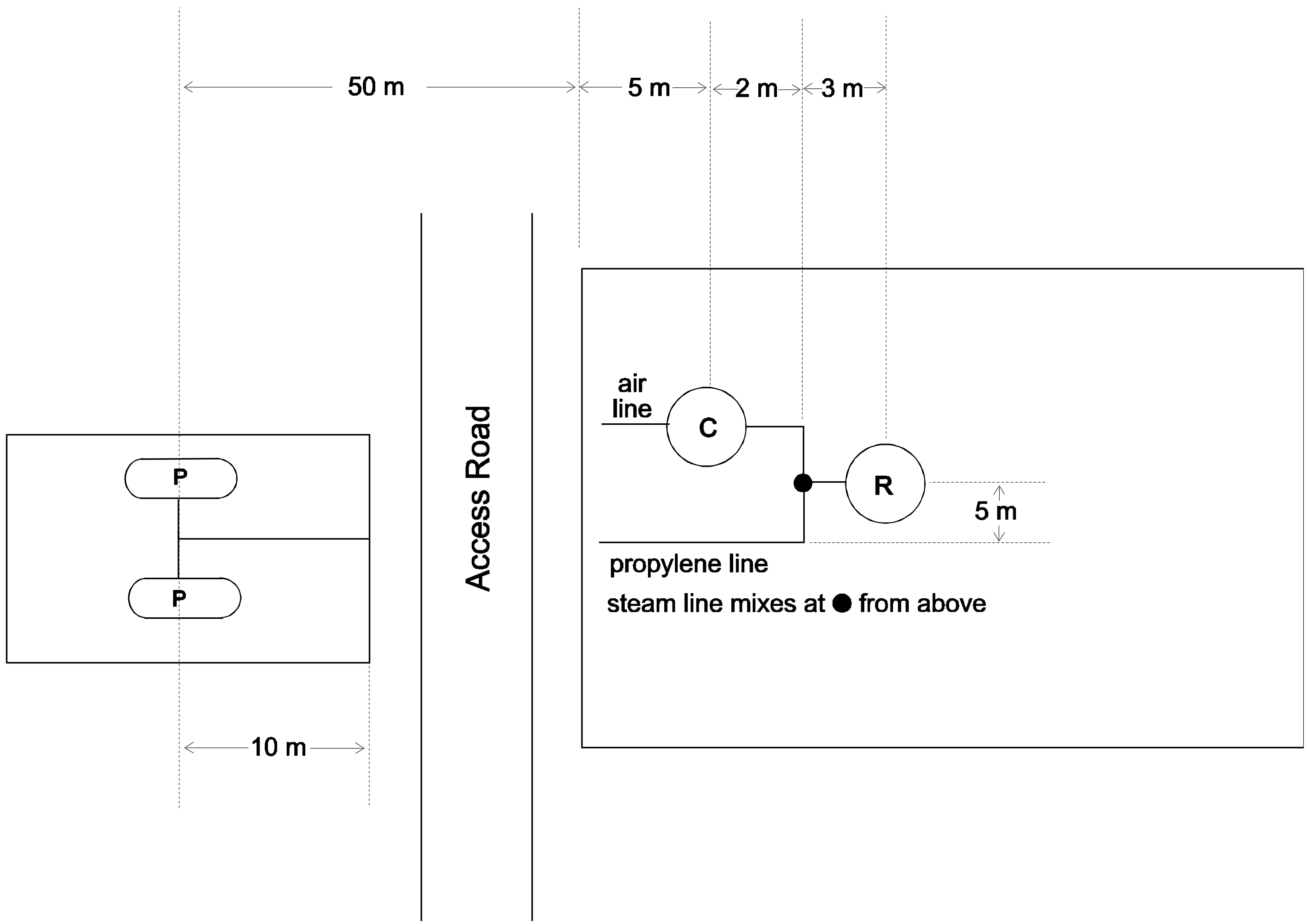


Figure 2: Partial Plot Plan forAcrylic Acid Production Feed Section

liquid storage needed – 2 tanks required, one for filling and one for feeding – assume 70% full with liquid) and determine the conditions for propylene storage. Propylene is to be stored as vapor/liquid mixture. Specify the elevation of the tank. We have a supply of centrifugal compressors used in other plants. The compressor curves are also attached (Figure 3). We would like the flexibility for 35% scale-up in the future.

2. **Optimization of the Dowtherm AÔ Loop.** (ChE 110 (fluids) and 111(heat)) The heat exchanger, E-301, must be designed in detail. The heat exchanger, pipes, and pump should be optimized together. *CAP* should include the costs of the pump, of the pipes, and of the heat exchanger. Operating costs should include the cost of pumping and the cost or credit for the heat removal medium in the heat exchanger. We also have a supply pumps used in our other plants which we would like to use in this plant. The pump curve is attached (Figure 4). This curve is for the pump having a 4 in impeller diameter. A 4.75 in impeller diameter can also be used. The pump efficiency is 80%, and is assumed constant. The pump and pipes should be sized to allow for 35% scale-up in the future. Equivalent pipe lengths should be determined from the attached plot plan (Figure 5). Pipe runs are at 4 m elevation off the ground, and you should add 90° elbows as necessary.

3. **Determination of Break-even Price for Crude Acrylic Acid.** (all classes) A Chemcad simulation for your best case should be presented. You may make any process modifications that improve the BEP, but a full optimization is not required. The break-even price (BEP) for crude acrylic acid product should be calculated. The best case is defined as the optimum case for “mini-designs” 1 and 2, above, plus any other changes to the process that you recommend. The break-even price for crude acrylic acid product is calculated as follows:

$$BEP = \frac{CAP\left(\frac{A}{P}, i, n\right) + \text{cost of reactants} + \text{operating costs} - \text{byproduct revenue}}{\text{kg acrylic acid in crude product}} \qquad (6)$$

where *CAP* is the installed capital cost for the entire feed and reaction sections, including the feed tanks.

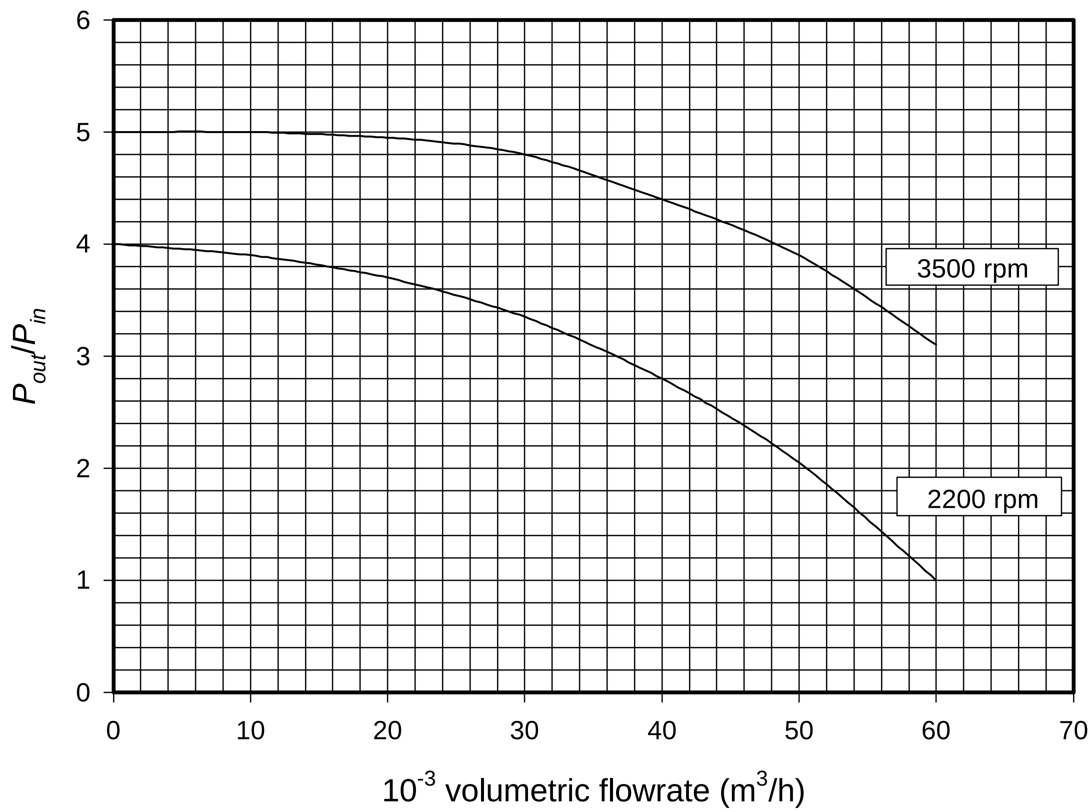


Figure 3: Compressor Curves for C-301

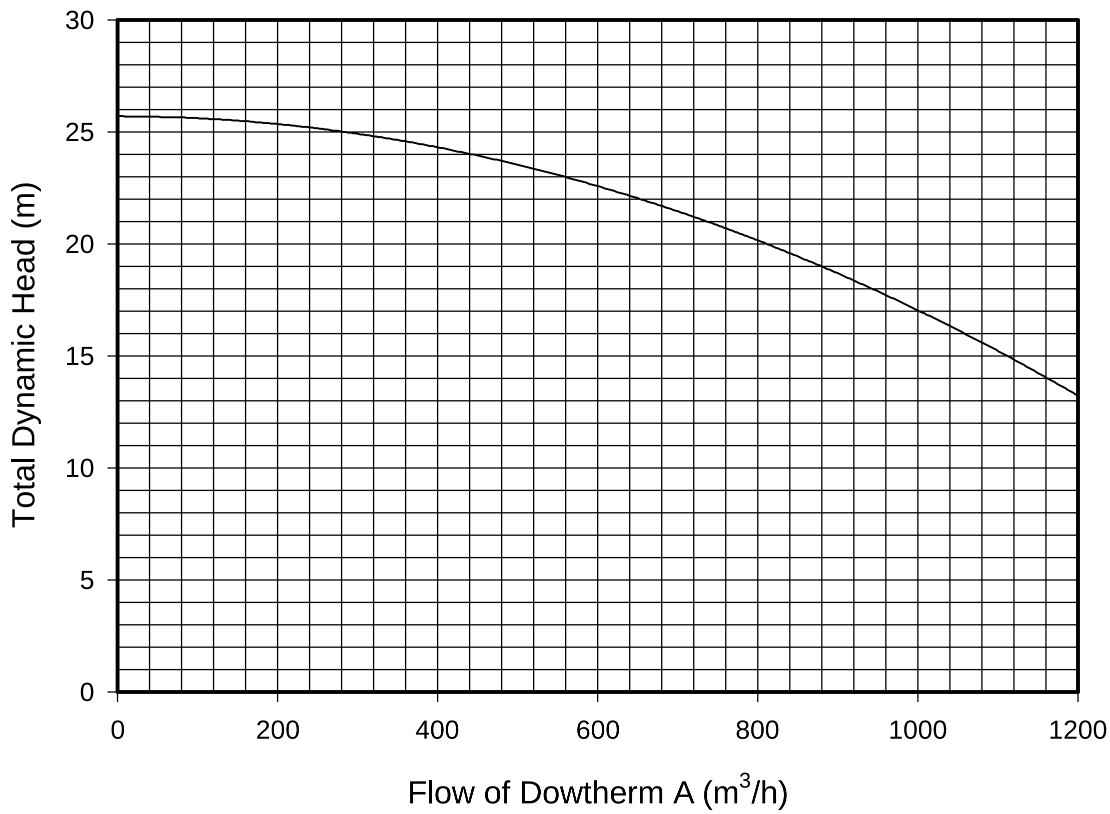
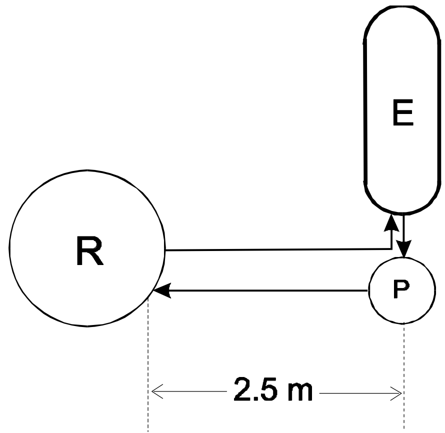
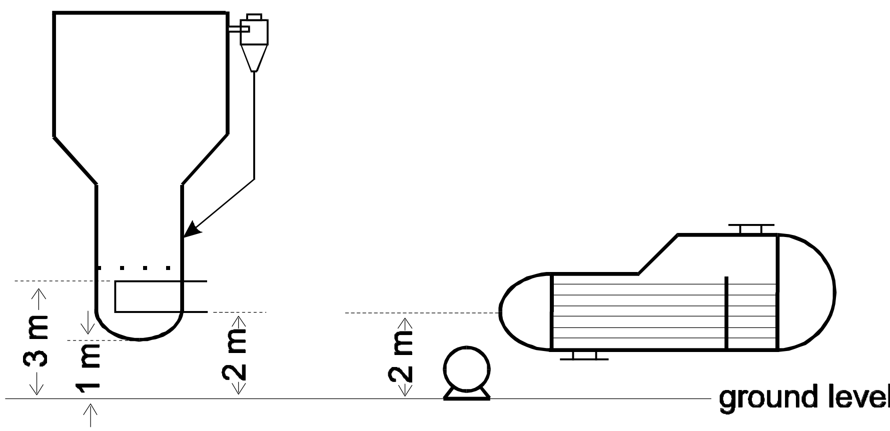


Figure 4: Pump Curve for the Dowtherm A Pump



Top View



Side View

Figure 5: Plot Plan for Dowtherm A™ Loop

Cost Data

Raw Materials

Propylene (polymer grade)	see *Chemical Marketing Reporter*

Utility Costs

Low Pressure Steam (618 kPa saturated)	\$6.62/1000 kg
Medium Pressure Steam (1135 kPa saturated)	\$7.31/1000 kg
High Pressure Steam (4237 kPa saturated)	\$8.65/1000 kg
Natural Gas (446 kPa, 25°C)	\$3.00/GJ
Fuel Gas use this price for fuel gas credit	\$2.75/GJ
Electricity	\$0.06/kW h
Boiler Feed Water (at 549 kPa, 90°C)	\$2.54/1000 kg
Cooling Water available at 516 kPa and 30°C return pressure ≥ 308 kPa return temperature is no more than 15°C above the inlet temperature	\$0.16/GJ
Refrigerated Water available at 516 kPa and 10°C return pressure ≥ 308 kPa return temperature is no higher than 20°C	\$1.60/GJ
Deionized Water available at 5 bar and 30°C	\$1.00/1000 kg
Waste Treatment of Off-Gas	incinerated - take fuel credit

Equipment Costs (Purchased)

Piping	\$/m = 5.0 (diameter, in)
Valves	\$100 (flow diameter, in)$^{0.8}$ for control valve with orifice plate, double the price
Pumps	\$630 (power, kW)$^{0.4}$
Heat Exchangers	\$1030 (area, m^2)$^{0.6}$ add 25% additional for boilers or evaporators
Compressors	\$770 (power, kW)$^{0.96}$ + 400 (power, kW)$^{0.6}$
Turbine	\$2.18$\times 10^5$ (power output, MW)$^{0.6}$ assume 65% efficiency
Fired Heater	\$635 (duty, kW)$^{0.8}$ assume 80% thermal efficiency assume can be designed to use any organic compound as a fuel
Vessels	\$$[1.67(0.959 + 0.041P - 8.3\times 10^{-6}P^2)]\times 10^z$ $z = (3.17 + 0.2D + 0.5 \log_{10}L + 0.21 \log_{10}L^2)$ D = diameter, m $0.3 \text{ m} < D < 4.0 \text{ m}$ L = height, m $3 < L/D < 20$ P = absolute pressure, bar
Reactor	assume to be \$5 million
Storage Tank	\$$1000V^{0.6}$ V = volume, m^3

Equipment Cost Factors

Pressure Factors

Pressure (absolute)	< 10 atm, 0.0 10 - 20 atm, 0.6 20 - 40 atm, 3.0 40 - 50 atm, 5.0 50 - 100 atm, 10	does not apply to turbines, compressors, vessels, packing, trays, or catalyst, since their cost equations include pressure effects

Material Factors

Carbon Steel	0.0
Stainless Steel	4.0

Total Installed Cost = Purchased Cost (4 + material factor + pressure factor)

Heat Exchangers

For heat exchangers that do not have to be designed in detail, use the following approximations for heat transfer coefficients to allow you to determine the heat transfer area and heat exchanger cost:

situation	***h* (W/m²°C)**
condensing steam	6000
condensing organic	1000
boiling water	7500
boiling organic	1000
flowing liquid	600
flowing gas	60

Other Information

You should assume that a year equals 8000 hours. This is about 330 days, which allows for periodic shutdown and maintenance.

Unless specifically stated in class, the information in this document is valid for this project only. Any information in the sophomore projects not specifically stated in this document is not valid for this project.

Deliverables

Each group must deliver a report written using a word processor. Three identical copies should be submitted, one for each instructor. The written project reports are due by 11:00 a.m. Thursday, December 4, 1998. Late projects will receive a minimum of a one letter grade deduction.

The report should be clear and concise. For the correct formatting information, refer to the document entitled *Written Design Reports*. Any report not containing a labeled PFD and a stream table, each in the appropriate format, will be considered unacceptable. PFDs from CHEMCAD are generally unsuitable unless you modify them significantly. When presenting results for different cases, graphs are superior to tables. For the optimal case, the report appendix should contain details of calculations that are easy to follow. There should be separate appendices for each “mini-design.” These may be hand written if done so neatly. Calculations that cannot be easily followed will lose credit.

Since this project involves three “mini-designs,” it is suggested that the report be organized as follows. There should be a general abstract and introduction. Then, there should be a results section followed by a discussion section for each “mini-design.” General conclusion and recommendation sections should follow. At a minimum, there should be an appendix for each of the three “mini-designs.” With this organization, there is no need for a separate section of the report for each class, as suggested in the document entitled *Written Design Reports*.

Each group will give an oral report in which the results of this project will be presented in a concise manner. The oral report should be between 15-20 minutes, and each group member must speak. A 5-10 minute question-and-answer session will follow. Refer to the document entitled *Oral Reports* for instructions. The oral presentations will be December 4, 1998, from 11:00 a.m. to 3:00 p.m., and possibly December 5, 1998, from 11:00 and to 1:00 pm. Attendance is required of all students during their classmates’ presentations (this means in the room, not in the hall or the computer room). ***Failure to attend any of the above required sessions will result in a decrease of one-letter grade (per occurrence) from your project grade in ChE 110, ChE 111, and ChE 142***.

Groups

You may do this projects in a group of three or four. You should select your own groups. Since there are 31 students doing the project, there will be eight groups. Seven groups will have four members and one group will have three members.

Revisions

As with any open-ended problem (i.e., a problem with no single correct answer), the problem statement above is deliberately vague. The possibility exists that, as you work on this problem, your questions will require revisions and/or clarifications of the problem statement. You should be aware that these revisions/clarifications may be forthcoming.